



chain nodes :

7 8 10 11 12 18 19 20 21 24 25 26 27 28 35 36 38 39 40 46 47 48 49 50
51 52 53 54 55 56 57 58 59 60

ring nodes :

1 2 3 4 5 6 9 13 14 15 16 17 29 30 31 32 33 34 37 41 42 43 44 45

chain bonds :

1-10 2-11 3-12 4-7 5-8 6-24 9-24 12-25 13-18 14-19 15-28 16-20 17-21 25-26 25-27
29-38 30-39 31-40 32-35 33-36 34-50 37-50 40-52 41-46 42-47 43-51 44-48 45-49
53-54 53-58 53-59 53-60 54-55 54-56 56-57

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-17 9-13 13-14 14-15 15-16 16-17 29-30 29-34 30-31
31-32 32-33 33-34 37-45 37-41 41-42 42-43 43-44 44-45

exact/norm bonds :

3-12 6-24 9-24 12-25 25-26 31-40 34-50 37-50

exact bonds :

1-10 2-11 4-7 5-8 13-18 14-19 15-28 16-20 17-21 25-27 29-38 30-39 32-35 33-36
40-52 41-46 42-47 43-51 44-48 45-49 53-54 53-58 53-59 53-60 56-57

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-17 9-13 13-14 14-15 15-16 16-17 29-30 29-34 30-31
31-32 32-33 33-34 37-45 37-41 41-42 42-43 43-44 44-45 54-55 54-56

G1:S02

G2:C,O,S,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS 11:CLASS
12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom
34:Atom 35:CLASS 36:CLASS 37:Atom 38:CLASS 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom
44:Atom 45:Atom 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

```
    containing 29
    containing 53
node mappings:
  26:55  25:54  3:31
```